

Thiophene, 3,4-dichlorotetrahydro-, 1,1-dioxide

Other names:	DAC PRD 3,4-Dichlorosulfolane 3,4-Dichlorotetrahydrothiophene 1,1-dioxide 3,4-Dichlorothiolane 1,1-dioxide Dichlorothiolane dioxide DAC PRO PRD PRD experimental nematocide Thiophene, tetrahydro-3,4-dichloro-, 1,1-dioxide NSC 13391 NSC 27866 NSC 35959
Inchi:	InChI=1S/C4H6Cl2O2S/c5-3-1-9(7,8)2-4(3)6/h3-4H,1-2H2
InchiKey:	JCUQWSIALJCIEE-UHFFFAOYSA-N
Formula:	C4H6Cl2O2S
SMILES:	O=S1(=O)CC(Cl)C(Cl)C1
Mol. weight [g/mol]:	189.06
CAS:	3001-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-474.02	kJ/mol	Joback Method
hf	-567.19	kJ/mol	Joback Method
hfus	20.42	kJ/mol	Joback Method
hvap	50.85	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.630		Crippen Method
mcvol	108.930	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
tb	403.22	K	Joback Method
tc	604.21	K	Joback Method
tf	288.95	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.02	J/mol×K	403.22	Joback Method
cpg	194.90	J/mol×K	436.72	Joback Method
cpg	205.22	J/mol×K	470.22	Joback Method
cpg	215.00	J/mol×K	503.72	Joback Method
cpg	224.23	J/mol×K	537.22	Joback Method
cpg	232.94	J/mol×K	570.71	Joback Method
cpg	241.11	J/mol×K	604.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3001578&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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